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A NATIONAL COMPUTING ENVIRONMENT FOR ACADEMIC RESEARCH

ORIGINAL

Prepared Under the Direction of
Marcel Bardon

COMPLETED

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by the NSF Working Group on Computers for Research
Kent K. Curtis, Chairman

National Science Foundation

July, 1983

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The views, budget projections and recommendations expressed herein are those of the participants in this study and do not necessarily imply endorsement of the National Science Foundation.

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Table of Contents

Page

Executive Summary 1

I. The Role of Modern Computing in Scientific and Engineering Research with Special Concern for Large Scale Computation 3

Background 3

A. Summary of Current Uses and Support of Large Scale Computing for Research 5

B. Critique of Current Facilities and Support Programs 7

C. Unfilled Needs for Computer Support of Research 8

II. The Role and Responsibilities of NSF with Respect to Modern Scientific Computing 11

III. A Plan of Action for the NSF: Recommendations 15

IV. A Plan of Action for the NSF: Funding Implications 21

Bibliography 25

Appendix

Large-Scale Computing Facilities 27

Executive Summary

Computing facilities have a decisive effect on the kind of research which is done by academic scientists and engineers. During the 1950's and 1960's, the Government encouraged the growth of computing in research, research methods were transformed in discipline after discipline, and the U.S. enjoyed a large, ever-widening lead in quantitative research and modelling complex phenomena. In the 1970s Government support slackened and academic computing facilities no longer kept pace with advancing technology. During this time, advances in computer technology introduced minicomputers, microcomputers, automated measuring instruments and a variety of other computer dependent tools into academic laboratories; but academic researchers fell behind their industrial counterparts in obtaining and using the rapidly advancing computer technology. American universities installed no supercomputers and although two disciplines, atmospheric sciences and magnetic fusion energy sciences, established national computing facilities for their research, only a few scientists in other disciplines could gain access to supercomputers anywhere. The effect on academic science was not immediately apparent but scientists gradually realized that lack of opportunity to use sophisticated computing technology directs academic research away from those areas which demand it. This leaves vital fields unexplored and impoverishes American science. The lack of opportunity to properly train graduate students is of particular concern.

There are many organizations, both private and public, active in computer-related research and education. For example, during the last few years NSF and other research supporting agencies have placed special emphasis upon improving academic research instrumentation. Some of these funds have been used for small computers. Also, computer manufacturers and other private sources are increasing their contributions to academic science and education, especially for computer-based activities. Four universities have installed supercomputers with assistance from CDC, Cray Research and Denelcor, but in general, support remains inadequate in all disciplines. In those disciplines that attempt to fund computing through individual research grants, access to large-scale computing remains minimal.

In December, 1982, the National Science Foundation issued the report of the Panel on Large Scale Computing in Science and Engineering, Peter D. Lax, Chairman, [1] which urged the Federal government to take measures promptly to stem the erosion of American leadership. In its report, the Lax Panel stated:

> "Current and feasible supercomputers are extremely powerful scientific and engineering tools. They permit the solution of previously intractable problems, and motivate scientists and engineers to explore and formulate new areas of investigation. They will surely find significant applications not yet imagined. For these reasons, the Panel believes that it is in the national interest that access to constantly updated supercomputing facilities be provided to scientific and engineering researchers, and that a large and imaginative user community be trained in their uses and capabilities."

In April, 1983, NSF organized an internal working group on computers for research to help develop an appropriate course of action for the Foundation to meet the computing needs of academic science and engineering. The members of this group consulted with scientists in their respective disciplines and drew upon their own experience as program directors to estimate the needs in their areas of competence. On May 23, 1983, NSF held a workshop with thirteen scientists from diverse disciplines to define the needs better, especially for large-scale computing and networking. The working group also consulted many earlier studies, met with NSF advisory committees and individual scientists, and drew upon other advice from the scientific communities. This led to six principal conclusions:

- The attitude toward computers for research marks a generation gap in the community of scientists. Older scientists may use, or have their graduate students use, computers for a variety of measurement and analysis tasks but consider the role and importance of computers to be limited. Younger scientists, who grew up with computers as part of their culture, view them quite differently.

- A large gap exists between need and available support for minicomputers, attached processors, workstations, high precision graphics, local area networks and other local facilities required as part of the researchers' and graduate students' daily working environments.

- There is an immediate need to make supercomputers more available to academic scientists and engineers. The actual magnitude of the requirement is difficult to assess because lack of opportunity has artificially depressed the level of activity but an estimate of the near term need is for ten systems including an advanced vector computer at the National Center for Atmospheric Research.

- Computer networks are necessary to link scientists, wherever they are, to large-scale computing resources and to each other. Development and use of such networks should be encouraged.

- Science has passed a watershed in using computers for research. Computers are no longer just tools for measurement and analysis but large computers, in particular, have become the means for making new discoveries. Very important lines of inquiry exist which require computing capability 100 to 1000 times greater than any now in prospect. Academic research in computer architecture, computational mathematics, algorithms, and software for parallel computers should be encouraged to increase computing capability.

- There is competition among computer manufacturers in education and research. This is resulting in favorable terms for educational institutions to acquire computer equipment and offers NSF an opportunity to leverage its funds.

One other important observation emerged from the Working Group's studies. Academic institutions are on the threshhold of a personal computer revolution, led by a few institutions such as MIT, Brown and Carnegie-Mellon and assisted by some computer vendors, which is putting computing power comparable to large computers of the 1960's in the hands of every student. Although this has deep significance, especially for undergraduate and precollege education, the Working Group did not attempt an analysis of this phenomenon but focussed its attention on research and graduate education.

To meet the needs of U.S. academic research and graduate student training it is recommended that NSF should:

1. Develop and coordinate programs in this area with other federal agencies and with private performers and supporters of computer related research and education such as the computer manufacturers, the Semiconductor Research Consortium, Inc. (SRC), the Microelectronics and Computer Technology Corporation (MCC), and other private research performers.

2. Greatly increase its support for local scientific computing facilities, including:
    - workstations for individuals or small groups of scientists, e.g., microprocessors, graphics, data storage capability, terminals, and printers;
    - computer systems for groups of researchers and students;
    - specialized facilities such as array processors, symbolic processors, experimental computer systems, and scientific data acquisition, storage, and dissemination centers;
    - local area networks of computers and workstations;

3. Encourage proposals to provide supercomputer services for academic research and science education and be prepared to support 10 supercomputer systems in the next three years;

4. Support networks linking universities and laboratories with each other and with supercomputer centers to provide access to facilities, file transfer capability and scientific communication;

5. Establish an advisory committee to advise the Foundation on policies and mechanisms for supporting computer services and networks and to provide oversight;

6. Support a vigorous program of academic research and training in the areas of advanced computer systems design, including building and evaluating experimental computer systems, and in computational mathematics, software and algorithms necessary to the effective and efficient use of computer systems.

The cost of this program is estimated to be:

	FY 84	FY 85	FY 86
Local Facilities	$45M	$91M	$107M
Supercomputers	$15M	$70M	$110M
Networks	$2M	$7M	$11M
Advanced Computer Systems and Computational Mathematics	$8M	$20M	$33M
Total	$70M	$188M	$261M

These sums are realistic for a near term national effort in academic science and engineering but even these investments would not provide computing facilities for academic researchers comparable to those at a typical national or industrial research laboratory. Boldness of execution will be critical to success in reasserting American leadership.

I. THE ROLE OF MODERN COMPUTING IN SCIENTIFIC AND ENGINEERING RESEARCH WITH SPECIAL CONCERN FOR LARGE SCALE COMPUTATION

Background

W. O. Baker writing in 1970 on the topic of "Computers as Information Processing machines in Modern Science"[1] observed:

> "Science, the vast producer and consumer of knowledge, has until lately held mostly to handwork for helping headwork. Of course, there have been mechanical aids to printing and publishing the record of scientific advance and more recently a host of ways of sensing and recording the measurements of scientific experiments by instruments. But in between the original observation and its insertion into the great corpus of scientific record there has persisted a wide, in some ways a primitive, personalized domain. Of course, this gap in mechanization does happen to contain a most awesome function of mankind—the ability to think. Now, suddenly, digital machines have come into this realm of the scientist, supplementing mysterious talents to perceive and to recognize patterns, to organize data, and, above all, to envision in the mind's eye new concepts and understanding."

Baker continued:

> "Likewise, the applications of science for the benefit of man through industry and government increasingly depend on the conception and design of large interacting systems, in which many of the elegant uses of computers that we have sampled must be combined in the most ingenious ways. Far from seeing a plateau or decline in the rate of progress in a golden age of science and technology, I see boundless opportunities through the use of logic machine systems to resolve the puzzles of cosmology, of life, and of the society of man."

Well over a decade later, as Baker foresaw, computing permeates every field of scientific endeavor in increasingly profound ways. Kenneth Wilson writing in 1982 on the "Role and Needs for Large Scale Computing for Theoretical Physics"[2] stated:

> "In conclusion, it is normal and reasonable that the computing demands for scientific simulation are prodigious, even by comparison with today's most powerful supercomputers. In fact, the whole area of scientific simulation in support of modern theoretical physics has barely been scratched; providing full access to theorists on the best of today's computers, can only be viewed as the beginning of many further stages of providing new levels of computing capability in support of ever more complex simulations. The complexity in simulation that can be handled numerically must keep pace with the growth in complexity that theorists are able to handle conceptually."

The use of modern computers in scientific and engineering research spans a period of only three decades, but it has been a dynamic period in which profound changes have taken place—and clearly the end is not in sight.

The period of the mid-50's through the 60's was one of significant change for research conducted in the academic environment; access to new tools—computers—was achieved. This was a period of the rise of campus computing centers in support of research and education. Institutional funds provided the bulk of the costs in achieving this objective but Government support (and occasionally industrial support) was often a deciding factor in an institution's decision to establish or upgrade its computing facilities.

Although most institutions chose to develop computing facilities on an institutional basis, others were developing shared facilities—one notable example being the Triangle Universities Computer Center (TUCC) involving cooperation among the University of North Carolina, North Carolina State University, and Duke University. One unique facility in the 60's, which provided services to researchers at many institutions, was the Western Data Processing Center at UCLA, a "large scale" center in its time established with support from IBM. IBM also provided support to UCLA in the late 60's together with support from NSF for a major campus computer facility featuring the IBM 360/91 computer, a "supercomputer" of this period. Similar large scale computing facilities featuring Control Data Corporation, IBM, or UNIVAC equipment and support were established at several other universities, also. A characteristic of these facilities was that they were developed for multidisciplinary use—providing computing services to researchers without regard to discipline as well as for educational use and often for administrative applications.

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[1] Baker, W.O. "Computers as Information-Processing Machines in Modern Science," Daedalus, Fall, 1970 pp. 1088-1120

[2] Report of the Panel on Large Scale Computing in Science and Engineering, Peter D. Lax, Chairman, December 26, 1982, Appendix II pp. 16-26

A different approach which provided extensive computing facilities for a single discipline or a group of closely related research activities was also started during the 1950's and 1960's. The U.S. Atomic Energy Commission encouraged extensive use of computers for management of large scale experimental facilities and data reduction in high energy physics. This was seminal work which greatly developed the application of computer technology to research. NSF organized the National Center for Atmospheric Research (NCAR) to be an intellectual center for major research efforts and a focal point for developing and housing the expensive and sophisticated research facilities required for effective progress in atmospheric research. The scientific computing facility was created within NCAR shortly thereafter. Computing resources were, and still are, allocated free of charge to NSF-supported atmospheric and oceanographic scientists in the universities and at NCAR.

Today, the computational power provided by NCAR is needed by atmospheric scientists and physical oceanographers to pursue the studies required for the advancement of the sciences. NCAR provides computing capability of a magnitude sufficient to support computations for extensive modeling and data analysis as well as storage and archive capacity for major data collections. The emphasis is on the best available, high-performance computers and support services tuned to this research.

The Scientific Computing Division at NCAR serves approximately 850 scientists through two CRAY-1A computers with IBM 4341 front-end systems, and a full set of graphics capabilities. Services provided to users from the staff of 100 individuals include: 24-hour per day operation throughout the year, consultation on systems, applications and numerical analysis, and large software libraries. Meteorological data bases are also archived and distributed.

The large computer facilities at the Department of Energy and NASA national laboratories also represent disciplinary-oriented facilities within the mission of their respective sponsoring agencies.

The Health Sciences Computing Facility at UCLA, supported by the National Institutes of Health, was a major computational research and services center in the 60's and early 70's. The Biomedical Statistical (BMD) Software packages, used extensively by researchers in many disciplines world-wide, originated at this center.

The horizons for the role of computing in scientific and engineering research broadened extensively with developments which began in the 60's to improve the access to computers. Remote access coupled with time sharing and interactive systems permitted users physically remote from the computer to make concurrent efficient use of a computer facility not only for creating and debugging programs on-line, but for production runs and subsequent analyses of data, often in an interactive mode. The sharing of computers does not in itself require remote access service; individuals can and, in many cases, do go physically to the site of the computer in order to carry out their research computing. Remote access, however, through specially designed computer-communication facilities, has led in a natural way to "networks" to improve computer access and user services for resource sharing. For example, remote users of the NCAR computing system access that system through the national communications network, UNINET. This is a low-cost, low error-rate, packet switching service with 177 nodes scattered throughout the Nation. In order for NCAR to provide the same level of computing capability as is provided to the 300 or so users at the Center, a plan of transmitting very large blocks of output data across the country at high speeds is being developed.

The period of the early 70's was a fertile one for coupling computers and research. Mini-computers became available and it was during this period that imaginative scientists in many disciplines began collaborating with computer scientists to make advances in research methodology. Achievements were many: Laboratory instrumentation became much more sophisticated as computers became an integral part of the system permitting monitoring and feedback on a real-time basis and coupling the researcher much more directly with the experiment. There was much exploration of the use of computer graphics. These sophisticated laboratory instruments were often in turn part of a local hierarchy, a network of computer facilities for more extensive data storage and analysis. A major computer research center for economics and management science was established at the National Bureau of Economic Research for advancing research methodology in those disciplines. A special project centered at Argonne National Laboratory (also supported by NSF) involved the collaboration of researchers on an international basis to create "certified" high quality mathematical software for a wide range of computers. This software and its successors are now widely used and have been incorporated as well in commercial software products.

In the early 70's some universities had the "supercomputers" of the period; however, by the middle 70's there were no supercomputers in universities. NSF support for campus computing centers was discontinued in FY 1972 and the research community turned to work which could be done with facilities available; those few academics who persisted in large scale computing invested large amounts of time and energy seeking time on facilities at Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory (LLNL) or in Europe.

Other changes were taking place as well: computing became an essential component of research in more and more disciplines and, technological developments which had led to the appearance of minicomputers later brought microcomputers and then supermicro's, VAX's and array processors. Consequently, academic departments or even individual research groups could, in effect, acquire their own computer centers. These developments coupled with a common practice of Federal granting agencies not to support the full cost of computer time led to a decentralization of campus computing. In many places, campus centers fell into disrepute as providers of services for research because of operating policies favoring small jobs, educational or administrative uses. During that same period, lacking Federal support for research instrumentation, academic facilities fell behind industrial laboratories in computing resources for research including minicomputers, workstations, graphics, etc. as well as supercomputers.

This image of undercapitalization of academic computing in the 1970's is confirmed by the data gathered in academic year 1976-1977 by John Hamblen and Carolyn Landis for EDUCOM [36]. They discovered that the total expenditures for computing in higher education was $991M in 1976-1977. Of that total only 7 percent came from Federal funds. 82 percent came from institutional funds and 11 percent from other sources. At major universities the proportion of Federal funds was slightly larger at 10 percent. By contrast, in 1966-1967 the proportion of computing expenditures at major universities provided by Federal funds was 34 percent. For higher education as as whole, it was 28 percent. Clearly, federal support did not keep pace with the expansion of need for academic computing.

It was in this milieu that the National Resource for Computational Chemistry (NRCC) was established. In their analysis of the Phase I operation of NRCC [35], the Ad Hoc Review Committee pointed out that the computational resources available through NRCC had been far too limited to have major impact. The capability which was provided (partial use of a CDC 7600) was not state-of-the-art; access to NRCC was never trouble free, and the available computing time was much too small. Furthermore, powerful minicomputers had recently begun to appear on the scene, and little of the research conducted at the very limited facilities of NRCC could not have been accomplished at local facilities, probably at lower cost and higher human efficiency. Since NRCC never did offer an advanced capability on the level of, say, NCAR, the failure of NRCC to produce any frontier research requiring such capability was a foregone conclusion. The chemistry community did not unite behind the vision of NRCC and its potential was never realized.

On the other hand, the DOE Magnetic Fusion Energy Computer Center (MFECC), dedicated to fusion physics calculations, was also established in the mid-1970's following recommendations of an Ad Hoc Panel on the Application of Computers to Controlled Thermonuclear Research. This center started operations in late 1975 with a CDC 6600 followed shortly by a CDC 7600. A review of requirements in early 1976 resulted in the procurement of a CRAY 1 within two years and a second CRAY 1 in 1981. The long-term commitment to supercomputers in this area, coupled with the development of a communication system for remote users and a strong user community, has led to a very successful utilization of this center.

The failure of NRCC and the success of MFECC depended critically on the non-availability or availability of supercomputers and the timidity or boldness of planning for each; the essential role of computing, and that of large-scale computing in particular, for the disciplines concerned was not at issue.

In recent years there have been many studies, culminating in the Lax Report [1], which call attention to a need for change in the policies of the Government vis-a-vis computing for academic research. In response to this concern, the National Science Foundation established an internal working group on computers for research in April, 1983, to help develop a plan of action for NSF. The members of this group consulted with scientists in their respective disciplines and drew upon their own experience as program directors to estimate the needs in their areas of research. On May 23, 1983, NSF held a workshop with thirteen scientists from diverse disciplines to define the needs better, especially for large-scale computing and networking. The working group also consulted with NSF advisory committees and individual scientists and drew upon other advice and publications from the scientific communities. This report presents a summary of the working group's conclusions and recommendations. A brief overview of large-scale computing facilities available for scientific and engineering research is provided in Part I.A. This overview includes national laboratories, universities and selected commercial service centers. More detailed information about the individual facilities appears in the Appendix. Part I.B. contains a critique of current facilities and support programs. In Part I.C., the type and amount of additional computing services needed is given. Section II. of the report analyzes the responsibilities of NSF for academic computing which result from the Foundation's charter and its relationship to other Federal agencies. Section III. contains recommendations for action by NSF and Section IV. provides budget estimates for carrying out those recommendations. A partial bibliography of relevant reports and other materials is attached, beginning on page 25.

I.A. Summary of Current Uses and Support of Large-Scale Computing for Scientific and Engineering Research

In this part, the supercomputer facilities of National Laboratories which offer access, in part, to academic researchers (within the constraints of the missions for which the facilities were established) are indicated. Brief descriptions of their major computer systems are given, as well as the research community served, communication access for remote users, charges, and plans for future expansion. Information is provided as well on three existing university supercomputer systems and three commercial service centers. A description is also provided of an ambitious plan to increase local computing capability at one major university, Cornell.

A more detailed description of each of these facilities is given in the Appendix.

From this list, it is clear that except for academic researchers in certain restricted groups, e.g., atmospheric sciences or NASA supported, or a few who can form collab-

FACILITY	MAJOR SYSTEM	RESEARCH USERS	CHARGES
NCAR	2 CRAY 1-A's	Atmospheric and Ocean Sciences	No charge to NSF users; $2,200 per prime CPU hour for others
MFECC	2 CRAY 1 1 CDC 7600	Magnetic Fusion Energy Community	No charge
LANL	(Open): 1 CRAY, 3 CDC 7600's, 1 CYBER 825	Government Agencies, Labs and Non-profit Institutions	$636 per prime CPU hour
NASA-Ames	CRAY 1-S CDC 7600	Computational Fluid and Aerodynamics	No charges to NASA grantees; $2,000 per CPU hour for CRAY
NASA-Goddard	CYBER 205	NASA-funded and NASA-project related	No charge to NASA grantees; $1,000 per CPU hour for others
NASA-Langley	CYBER 203	NASA and NASA-funded scientists	$1,300 per CPU hour
NASA-Lewis	CRAY 1-S	Principally Aero-dynamics-related	No charge for NASA-supported
Colorado State University	CYBER 205	University users and others	$2,000 per hour for university users
Minnesota	CRAY 1-A	University users and others	$2,000 per hour for University and non-profit; $3,000 per hour for others. Volume discount available.
Purdue	CYBER 205	University users	Not yet determined
Boeing	CRAY 1-S		
CYBERNET	CYBER 205	All	Variable
U. I. S.	CRAY 1-S	High-tech., insurance companies, etc.	Variable
Cornell	IBM 370-168 Several 4341's FPS AP-190L FPS 164	50-100 Cornell scientific users	Typical user rates: $20-40 per CPU hour (non-profit) for array processors; $500-$1,500 per hour on IBM hosts

orations with researchers at the Los Alamos or Livermore National Laboratories, there is no access to supercomputer facilities without substantial funds. The unit cost of acquiring and operating supercomputer facilities is very high, on the order of $10 million. It has not proven possible to accumulate these costs through recharges to individual research grants or contracts because too many competing interests interfere with the concentration of funds for computing. At the level of the research supporting agencies, confronted by inadequate research budgets, support of graduate students, research scientists and small laboratory instrumentation exhausts the available funds. At the level of the individual recipient of research support, funds granted for computing are recognized as inadequate and often diverted to other purposes. This has discouraged the development of computer-based research. Apparently, extraordinary measures are required to assure access to supercomputers. Dr. A. Trivelpiece, DOE, noted in his testimony to the joint hearings of the Subcommittee on Energy Development and Applications and the Subcommittee on Energy Research and Production of the House of Representatives Committee on Science and Technology on Tuesday, June 7, 1983, that in the Department of Energy's experience one must allocate computer time, not money. Otherwise, sufficient access to supercomputer facilities for research cannot be assured. NSF's experience is consistent with DOE's. NCAR, which allocates free time on its supercomputer facilities to meritorious atmospheric sciences research has been very successful in serving the academic atmospheric science community. Few other NSF supported scientists have been able to gain access and then only with great expenditure of effort.

In closing this section, reference should be made to the growing use of supercomputers by industry. Oil companies have turned to supercomputers for assistance with exploration for new deposits of oil and gas reserves and for tertiary recovery of oil deposits. Manufacturers of advanced microelectronic circuits, involving hundreds of thousands of logical elements on a chip, are using supercomputers to check circuit designs for completeness and consistency. Airplane manufacturers have used supercomputers for many years to assist with the analysis of aerodynamic flow around proposed designs and have found that computer analysis can greatly reduce the very expensive tunnel testing time required to perfect new designs. Even the movie and television industries have turned to supercomputers to create the elaborate visual effects that have appeared on recent films. The private sector has offered a new and substantial market for supercomputers in the past few years and it is expected that these applications will grow in number as the computing power of supercomputers increases to permit more realistic simulation of complex, three-dimensional, time-dependent phenomena.

I.B. Critique of Current Facilities and Support Programs

There is much positive to be said about the computer facilities and support programs currently available—particularly the efforts of communities of users, whether by discipline or by organizational entity, to develop computer facilities, networks, and services for resource sharing, and the efforts of the commercial sector as well to provide high quality computer-communication links. Nevertheless, important scientific and engineering research problems are not being attacked at present for lack of computer facilities with sufficient capacity and capability and appropriate access (network or otherwise).

To turn specifically to the concern for large-scale computation in scientific and engineering research, a closer examination of the present situation in regard to capacity, capability and access reveals many deficiencies. The DOD, DOE and NASA facilities are reserved for their respective contractors or at least for problems within the missions of these agencies. The NCAR computer facility is fully utilized by NCAR and the academic community in the atmospheric and related areas. University supercomputer facilities have been established only recently. User communities and the underlying financial bases are being developed. The latter is uncertain of accomplishment through individual research project grants. The machines are considered to be under-configured currently for many problems. This may also be a factor, in part, for their present underutilization. Furthermore, none of the existing university facilities is presently equipped to provide the services necessary to serve a large community of off-campus users. Aside from the hardware and software, this includes services such as remote consultation, training, etc.

The situation with respect to U. S. facilities for academic research is in marked contrast to that in some foreign countries, W. Germany, for example, where adequately configured machines are readily available to scientific researchers. Indeed, some U. S. researchers have actually traveled to foreign countries to perform large-scale computations that they were unable to perform here because of lack of access to national laboratory facilities or lack of funds to purchase supercomputer services. The fact that this inefficient and costly method of performing research was consciously chosen indicates the inadequancy of the situation with regard to access to large-scale computing facilities in this country. It also illustrates that the existing NSF mechanisms for support of computational science do not appear adequate to remedy this situation.

Computer networks are an important vehicle through which to improve the development and utilization of information and distributed computing resources. There are many existing networks, some of which (e.g., MFE) include nodes providing large-scale computing capacity. However, like most current supercomputer facilities, access to these networks is restricted to special communities. These communities do form important subsets of the total scientific community, so the existing networks do provide a substantial base on which to build. Unfortunately, sufficient motivation for extensions of the necessary scope and flexibility is unlikely to be generated from within existing networks.

Although the barriers to such extensions are mostly political, organizational and economic rather than technological, they are still sufficiently large to inhibit unilateral action.

An assessment of large-scale computing for scientific and engineering research is provided by the many studies and plans in the reports listed in the bibliography.

Thus, the vital role of computing in research, and especially the role of large-scale computation, is well established. Problems are now being addressed, as Professor Kenneth G. Wilson indicated, which require tens to hundreds of hours of computer time of computers operating at hundreds of millions of operations per second. In some problems, data in quantities measured in trillions of bits are analyzed using sophisticated computer graphics systems to augment human powers of analysis. Without computers these computations and analyses would be completely impossible to carry out.

While *capacity*[3] is one concern, a greater concern for the future is *capability*.[4] Some persons describe these as brute force and turn around time, respectively. At both the very low end (personal computers) and the very high end (supercomputers) capability is the limiting factor on the problems which can be solved. The elapsed time or scientists' waiting time must be realistic to make a line of research feasible. The participants in the Foundation-sponsored Workshop on Computers for Research on May 23, 1983, indicated several problems that they would like to solve but can not because of the capability of current computers. Among these were:

— (BIOLOGY) The simulation of a bi-layer membrane in contact with ions in water would permit tracing the paths determined by polypeptides for ion transport through the membrane. It is estimated that computational power of 1000 times a CRAY is needed for this fundamental problem of biological significance.

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[3] *Capacity* is defined as a measure of the volume of work a specified configuration can accomplish in a unit of time.

[4] *Capability* is defined as a measure of the highest degree of complexity or largest size of one job that a computer or network can process in some specified time frame.

- (CHEMISTRY) Chemical reactions can be modeled using the basic equations of quantum mechanics. To model reactions involving larger, more interesting, molecules, substantially more computational power is needed.
- (MATERIALS RESEARCH AND ELECTRICAL ENGINEERING) As dimensions get small in microelectronics, classical physics fails. Quantum mechanics is needed to model small-dimension physics for semiconductor devices.
- (CHEMISTRY AND MATERIALS RESEARCH) To understand catalysis on a surface, extensive calculations beyond present capabilities are required.
- (ATMOSPHERIC AND OCEAN SCIENCES) Turbulence calculations require three-dimensional simulations which can not be done with current computational capabilities.
- (ATMOSPHERIC AND OCEAN SCIENCES) Calculations for atmospheric modeling require finer resolution of grid points and longer time-scales; modeling ocean basins would require about 100 times the current capability.
- (EARTH SCIENCES) Modeling dynamic magnetic systems,—for example, to determine why the Earth's magnetic field reverses—requires capability beyond that currently available.
- (ENGINEERING) The computer capability does not yet exist for effective non-numeric processing required for robotics and for knowledge-based systems.
- (ASTRONOMY AND PHYSICS) Astrophysical problems such as modelling the processes by which stars are born require much greater computer capability than current supercomputers offer.
- (PSYCHOLOGY AND INFORMATION SCIENCES) Current computers are not sufficiently powerful to model a human's complete knowledge, even of one limited subject area.
- (ECONOMICS) Computer technology now limits the rigor and size of dynamic nonlinear economic modeling.

Strong research efforts in computer architecture, computational mathematics, algorithms and other aspects of computer research will be required to achieve the significantly increased computer capabilities required to address these future generations of research problems. A concerted effort is therefore needed to strengthen substantially academic research programs in computer systems—from which most significant advances have come—in this search for new computer architectures applicable to the scientific and engineering research problems of the future.

Supercomputers and large-scale networks represent only one end of the spectrum of capability needed by computational researchers. Many, if not most, scientific computations can be performed with tools of lower capability. These are tools which should be locally accessible to a researcher: campus mainframes, departmental minicomputers, personal workstations, etc. Indeed, with the advent of special-purpose processors, local facilities offer the most cost-effective and humanly efficient means of increasing both access and capacity, within the limits of their capabilities. Furthermore, adequate local facilities are absolutely essential for the success of any distributed large-scale computing system. Any examination of the overall needs of computational science must consider local facilities as an integral component of the total need.

Disciplines vary widely in the degree to which computer use has developed within the community. It can be seen that disciplines also vary widely in the mix of need for capacity across the spectrum of capability. Nevertheless, whatever the mix, the unmet need is substantial.

I.C. Unfilled Needs for Computer Support of Research

Many studies have documented the unmet needs for computer support of research in a qualitative fashion. Quantifying these needs is more difficult, especially with respect to large-scale computation. To assist in this effort, various information sources were utilized. One of these was a workshop held on May 23, 1983. The participants, who are listed on page 2, were computationally oriented scientists drawn from the whole spectrum of disciplines, representing not only academics, but also industry and the national labs. They were asked to consider the unmet needs in four areas:

- large-scale computing capacity
- local facilities
- networks
- new capability

Regarding the first, there is unanimous agreement that important science is not being done in this country due to lack of access to adequate supercomputer capacity. If an academic scientist does not belong to one of the specialized research communities with guaranteed access, it often requires heroic efforts to scrape together adequate access. For example, important astrophysical calculations essentially could not be performed in the U. S. because they did not fall into one of the areas (atmospheric sciences, magnetic fusion, etc.) covered by the specialized facilities, and the few university supercomputers were inadequately configured for the task. In this particular case, the researcher resorted to travelling to West Germany, where a collaboration with scientists having adequate supercomputer access allowed the calculations to be performed.

Needs for large-scale computing capacity will grow rapidly as more disciplines acquire computer experience. These needs may arise in unexpected ways. For example, the biology community has established a nucleic acid sequence data bank at Los Alamos to make this vital information generally available to researchers. Unfortunately, as the data bank grows large even the most elementary manipulations of it, such as finding all entries matching a given sequence, consume several minutes on current supercomputers. When multiplied by the many demands, the needed supercomputer capacity greatly exceeds that available to the data bank.

The available evidence indicates an urgent need to make a capacity equal to at least two adequately configured supercomputers available to the general scientific community immediately. The best projection is that as many as ten will be required to have any major impact on the total unmet need across all areas of science.

To keep the number ten in perspective, it is worth noting that the magnetic fusion energy community alone currently has access to two supercomputers, and the Los Alamos National Laboratory has five.

Other types of large-scale computing facilities are also important for various disciplines. The nucleic acid sequence data bank, cited above, is one example which is of interest to biology and chemistry. For computer research, and increasingly for other disciplines as they also engage in the design of special purpose computers, a service to fabricate custom-designed Very Large Scale Integrated (VLSI) circuits will be needed. The MOSIS facility, sponsored jointly by NSF and DARPA, is a prototype of such a service. Other specialized large-scale facilities will become important as computers are used more in research.

A network appears to be the only logical vehicle for making this capacity accessible to the general scientific community. Experience with existing networks (e.g., MFE net) has been very positive. Workshop participants were in general agreement that a network is an essential component of any response to unmet needs in large-scale computing. A network can also facilitate the interaction between scientists and promote the exchange of information, in addition to serving as a medium of communication between scientist and computer.

Regarding local facilities, there is agreement that they must be significantly strengthened, and that this must be undertaken for a balanced response to computational needs. Supercomputer access should be managed as a scarce resource. Indeed, any calculation which does not require supercomputer capability should be excluded from access to supercomputers and performed on other facilities.

Such calculations are most efficiently performed locally, and since such calculations will comprise the bulk of important scientific calculations, substantial local facility capacity is needed. Although funding patterns have changed radically in response to the shift toward decentralized local computing spawned by technological advances, funding levels have not kept pace with needs. All disciplines now experience unmet needs for local facilities.

The preceding discussion has dealt entirely with access to capacity. Scientific researchers also need access to machines of vastly higher capability. Factors of 1000 tend to be mentioned routinely. While factors of 10 are foreseeable with technological improvements, no one knows how to build a machine 1000 times faster than those currently available nor how to develop problem strategies or algorithms for them.

Thus, in contrast to the other unmet needs, the need for increased capability is the ultimate stumbling block. In all disciplines, progress in computational science will simply grind to a halt unless this impasse is resolved. Obviously, from a long term perspective this represents the most urgent need of all. Since it is also fundamentally a research problem, its resolution may be slow and painful; consequently it needs immediate attention.

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II. THE ROLE AND RESPONSIBILITIES OF THE NATIONAL SCIENCE FOUNDATION WITH RESPECT TO MODERN SCIENTIFIC COMPUTING

A. Introduction

The role and responsibilities of the National Science Foundation with respect to modern scientific computing must be defined within a larger context: the role and responsibilities of the Federal Government in research and development.

Substantial investments in basic research in all areas of science and engineering are widely recognized as essential for the long term health, prosperity and security of the Nation. It is also widely recognized that it is the responsibility of the Federal Government to provide the necessary investments in cases where there is insufficient incentive for the private sector to do so. This recognition is reflected by the increased attention now being focused on Government-wide support of basic research in general.

Within the overall Federal role, the National Science Foundation has the lead responsibility for basic research and science education conducted in academic institutions. By the National Science Foundation Act of 1950, as amended, the Foundation is authorized and directed to

> "...initiate and support basic scientific research and programs to strengthen scientific research potential and scientific education programs...in the mathematical, physical, medical, biological, engineering, social, and other sciences...
>
> and
>
> "...foster and support the development and use of computer and other scientific methods and technologies, primarily for research and education in the sciences..."

Thus, from both a general and a specific perspective, the Foundation has a mandate to assume a major responsibility with respect to computing for research and education in the sciences and engineering.

B. NSF as a Supporter of Access to Computer Capacity

Historically, the Foundation has interpreted this responsibility to include programs designed to promote access to and improve the capacity and capability of whatever computing facilities may be necessary for the solution of fundamental problems in basic research as well as education in the use of such facilities.

For example, from 1957 to 1972, the Foundation awarded grants to help initiate and expand computing facilities for education and research at colleges and universities. In that era, large mainframe computers in campus computing centers were *the* research instruments for the comparatively few computationally-oriented scientists, including the practitioners of the then-novel discipline of computer science. This program was instrumental in insuring that adequate computational facilities were available to these scientists. The program had a significant educational component as well. It played a major role in the development of a body of computer-literate individuals in the U.S. more than a generation before any other country. The focus of the program was always stimulation rather than sustenance, and few institutions received more than one award. The program was finally discontinued when it was perceived that the providing of computer services had become sufficiently incorporated into the normal operation of major research universitities that special Foundation assistance was no longer required. The Foundation then reverted to supporting scientific computation by the distribution of funds for the purchase of computing services through individual research grants.

Another illustration is provided by the special computing facilities that have been created on occasion by the Foundation in response to specific perceived needs. The two notable examples are NCAR and NRCC. The former has, of course, been very successful in its mission, while the latter was not successful, for reasons mentioned previously. These two contrasting examples point out the importance of careful planning and highlight the danger of proceeding with inadequately configured facilities. A submarginal response to a specific need may be worse than no response at all.

The trend toward a more decentralized environment for scientific computing which was sparked by the minicomputer and accelerated by the microcomputer is generally a very positive direction. These devices offer a quantitative leap in both the access and capacity that can be made available to the scientific community for a given investment. The supermicro of today has the capability of the most powerful mini of a few years ago, while a modern mini with attached processor can put the equivalent of a CDC 7600 into the hands of an individual department or research group. Recognizing the cost-effectiveness of this trend, many areas of the Foundation have already been quite receptive to proposals requesting assistance in the purchase of minicomputers or microcomputers. This receptive posture should be extended to the Foundation as a whole. The unmet need is very great, as indicated in section I. Furthermore, minicomputers and microcomputers for scientific research have no fundamental distinction from other equivalent cost instruments for scientific research routinely requested from the Foundation. The only difficulty with adopting such a posture is that it can only increase the competition for already scarce instrumentation resources.

C. NSF Policy vis-a-vis Large-Scale Computing

While increased support for the acquisition of minicomputers and microcomputers would go a long way toward alleviating many needs for increased access and capacity, such a policy can have no effect on unmet needs for access to computing systems of the highest capability. These systems are known generically as supercomputers. At any given time, only a small fraction of basic research problems might truly need supercomputer capabilities. However, in many disciplines, it is precisely these problems which are encountered at the frontiers of progress.

The current situation in the U.S. with regard to supercomputers is far from optimum on almost every count. Supercomputers are manufactured by only a few vendors. The total number of machines is quite small. None of them is easily accessible by a member of the general scientific research community, and most of them are not accessible by that community at all. In particular, only four supercomputers presently may be found at universities.

It has also become evident that although the U.S. has always been the leader in the development and use of supercomputers, that leadership is being challenged on a number of fronts.

The role and responsibilities of the National Science Foundation with respect to the special problem posed by large-scale computing and supercomputers must also be defined within the overall Federal role. Several Federal agencies have already proposed attacks on various facets of this problem.

The Department of Defense, through DARPA, has established a program aimed at the development of strategic computers to meet specific DOD objectives. While the goal will not be machines for general-purpose scientific computing, the program will undoubtedly provide a great stimulus for certain aspects of computer science and engineering.

NASA is planning to develop a new Numerical Aerodynamic Simulator (NAS). NAS will include a specialized large-scale computing system that will perform calculations required to design aircraft and significantly reduce wind tunnel and flight testing. In space research, NASA expects its computational workload to increase from one to ten billion operations per second. To meet this need, the Massively Parallel Processor has been developed and processing research will begin this summer. NASA has large-scale computational capacity at the NASA centers. These facilities are dedicated for use by NASA scientists and engineers, NASA contractors, and NASA-funded researchers.

The Department of Energy is investigating ways to make its own large-scale computing facilities more accessible to qualified researchers who need such capabilities. They also are examining how the Federal Government as a whole can stimulate the commercial development of supercomputers. Vendors generally agree that the most important first steps are for the Government to maintain a "friendly customer" attitude and to provide industry with realistic projections of minimum Government needs in the area. Since future needs in capability probably will require some radical departures from current designs, the "friendly customer" attitude might extend to experimental prototypes which show reasonable promise of achieving breakthroughs in capability.

In view of the Foundation's responsibility for basic research and education in science and engineering, its role with respect to large-scale computing and supercomputers should be to maintain strong programs designed to provide:

- support of basic research and science education in universities in computational mathematics and advanced computer concepts including software, algorithms, architecture, subsystems, and components;
- support of basic research in problems that require large-scale computing across all areas of science and engineering;
- training of scientists and engineers in the concepts, design, and use of large-scale computing systems;
- assured access for researchers and graduate students to large-scale computing facilities.

If the words "large-scale" are deleted, the preceding four statements provide an effective summary of the role of the National Science Foundation with respect to modern scientific computing in general. The Foundation recognizes that item four is crucial for the success of items two and three, and has assigned a high priority to resolving problems of access at all levels of capability.

These responsibilities of the Foundation with respect to scientific computing are not shared with any other agency. In particular, the problem of assured access to large-scale computing for academic scientific research is not addressed at all by the DARPA strategic computer program, and only slightly by the NASA and DOE programs. Thus, the Foundation should assume the lead role in the resolution of this problem in accordance with its responsibilities.

Supercomputer systems probably will never again be commonplace on university campuses. The image of a supercomputer in every academic computing center appears quite unrealistic. The capital and operating costs of such a facility are simply too great relative to the average need that will be generated from within a single university.

Given that this situation is likely to persist into the foreseeable future, attempts to support large-scale scientific computing solely by the distribution of funds through research grants probably are doomed to founder on the problem of access. The Foundation's experience has shown that academic institutions are often reluctant to spend grant funds for off-campus services, especially in computing. In addition, both NSF staff and researchers, when faced with budget restrictions, often sacrifice computer time budgets first as being most easily postponed. In brief, willingness on the part of the Foundation to provide funds for large-scale computation in research grants is, in itself, insufficient to insure that scientifically pressing large-scale computations can, in fact, be done. Insuring access to large-scale computing facilities requires more drastic action ranging from contracting for large blocks of time with existing suppliers to creation of dedicated facilities. The Foundation has the responsibility to consider special solutions of this problem, including the possible role of large-scale networking.

The fact that special solutions are required indicates that access to large-scale computing for scientific research is a special resource. Inevitably, this means that it will be a scarce resource, and it should be treated as such. The goal of the Foundation should be to insure that a scientific researcher has access to precisely the capacity and capability needed for the particular problem at hand. Since only a small fraction of the time will this imply supercomputer capability, any policy which attacks only this aspect of the problem makes little sense, either scientifically or economically. There are substantial needs at all levels of accessibility, capacity, and capability, across all disciplines. All these needs must be addressed for maximum results to be obtained.

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III. A PLAN OF ACTION FOR THE NSF: RECOMMENDATIONS

A. Introduction

Section I. of this report has shown that the presence or absence of computing facilities has a decisive effect on the kind of research which is done. The failure of the U.S. to provide supercomputer facilities for academic research throughout the 1970's and early 1980's discouraged the development of U.S. science in the direction of large-scale, complex modelling except in those disciplines such as atmospheric sciences, fusion research or aerodynamics which specifically provided supercomputers for their researchers. Further, there are strong indications from the scientific community that urgent action is needed. For example the initiative of Nobel prize-winner Professor Kenneth G. Wilson, Cornell University, whose current work has its principal focus on numerical modelling of physical phenomena and who is publicly urging greatly increased support for computer-based research [34], is a signal that we can no longer procrastinate. U.S. scientific and engineering research is being blunted by the lack of appropriate computing power.

During this same period, the U.S. has not provided the wide variety of computing services its academic scientists need to keep them in step with modern technology. Supercomputers are only one component of the collage; and minicomputers, attached processors, personal workstations, high resolution graphics, symbolic processors, local area networks, etc. are indispensable for modern research productivity. Industry, which recognized this for its own R&D, makes large investments each year for its scientists and engineers to supply computer equipment, software and support personnel. The Federal Government needs to do the same for academic research.

Section III. of this report presents recommendations for a plan of action for NSF. The Foundation should act on four levels:

a. increase support for local computing facilities;

b. support supercomputer services and access thereto for academic scientific and engineering research and education;

c. assist with the formation and use of appropriate computer communications networks;

d. support academic research in advanced computer systems design and computational mathematics to improve our computational capability for solving problems beyond the reach of todays supercomputers.

Each of these is treated in turn.

B. Coordination

As has been noted several times, there are many active participants in computer-related research at all levels. Several Federal agencies are involved in or support computer-related research relevant to their missions. The computer manufacturers and some other companies such as Bell Laboratories, General Electric, Exxon, Xerox and General Motors have substantial in-house research programs and help support academic research and education. The SRC and MCC are supporting and conducting research, respectively, in relevant areas and several nonprofit corporations such as RAND, Draper Laboratories, SRI International, and MITRE are research performers. Also, there is an increasing number of companies utilizing supercomputers in such diverse fields as oil exploration, VLSI circuit design, and making movies. All of these activities depend upon academic research for ideas and for trained people able to contribute effectively to the goals of the organization. In such a dynamic environment coordination is essential. This leads to the first recommendation:

> **Recommendation 1:** NSF coordinate its programs in this area with other Federal agencies and with private supporters and performers of computer-related research and education.

C. Local Facilities

Almost all scientists and engineers need a wide variety of computer services whether they use supercomputers or not. At or within close proximity of their everyday working environment, researchers need to be able to write and debug programs, store, transform, and display data, perform computations and statistical analyses, explore mathematical strategies for modelling physical phenomena, communicate with collaborators and perform many other essential professional tasks. Interactive systems are especially useful for these purposes. On them, researchers can test and make use of experimental systems. Industrial scientists and engineers have found these tools indispensable for their work. For academic science and engineering, NSF must increase its support for this purpose. The amount and type of local facilities needed will vary greatly among disciplines, types of research and working patterns of individuals. This leads to the second recommendation:

> **Recommendation 2:** NSF greatly increase its support for local scientific computing facilities, including:

- workstations for individuals or small groups of scientists, e.g., microprocessors, graphics, data storage capability, terminals, and printers;
- computer systems for groups of researchers and graduate students;
- specialized facilities such as array processors, symbolic processors, experimental computer systems, and scientific data acquisition, storage, and dissemination centers;
- local area networks of computers and workstations.

D. Supercomputer Facilities

Since 1970, the Foundation has provided supercomputer facilities for only one community of researchers, those in the atmospheric and physical oceanographic sciences. Generally, scientists in other disciplines have been able to use supercomputers only if they performed research of relevance to the national laboratories such as Los Alamos, Livermore, NASA/AMES or Kirtland Air Force Base, or formed collaborations with foreign scientists to gain access to supercomputers in Europe.

The use of supercomputers is indispensable to the atmospheric and oceanographic scientists. For example, for the study of turbulence they need computers which are still five times more powerful than the CRAYs they have installed. This has led NSF to develop a plan for installing an Advanced Vector Computer at NCAR in FY 1985 which will provide that needed capability. Other disciplines have similar needs and, in some cases, problems which are even more demanding.

There is no question about the existence of problems in many fields of science and engineering which require supercomputers, nor about the presence in universities of researchers interested in these problems and capable of such investigations. However, it is difficult to estimate the amount of supercomputer capacity needed because lack of opportunity has depressed this kind of research activity to artificially low levels. As a result, we cannot easily gauge either the immediate unfilled need or the rate of growth which should be allowed if opportunity were to arise. At the Foundation-sponsored workshop on May 23, 1983, scientists in each of several disciplines described the situation in their field, and estimated immediate requirements and growth rates on the basis of their knowledge of the research problems and talent available. They noted that it will take a strong sustained commitment to large-scale computing by the Foundation to persuade scientists to invest their time and effort, sometimes involving years, in preparing programs for supercomputers. Nevertheless, they could identify problems and colleagues ready to work, some of them now seeking time at foreign research laboratories. The discussions of the May 23 Workshop led to the conclusion that an immediate need exists for NSF to provide two supercomputers in addition to the Advanced Vector Computer at NCAR, and that growth by a factor of five in the following two years should be supported. This leads to the third recommendation:

> **Recommendation 3:** NSF encourage proposals to provide supercomputer services for academic research and education in science and engineering and be prepared to support 10 supercomputer systems within the next three years.

E. Networks

1. Need for a Network

Supercomputer facilities are scarce resources. Few laboratories or universities are likely to have such state-of-the-art systems as local research tools. Rather, as in many other fields needing expensive research equipment, supercomputers will be installed as centralized facilities at a few locations. They will be open to use for meritorious research (determined by peer review) by a geographically widely scattered community of users. While some scientists may need to be physically present at the facility to carry out research projects, most will find that travel to a distant site is a highly inefficient use of their time, as well as a barrier to graduate student involvement in the research.

Remote access to supercomputers is a realistic option with existing telecommunications technology. This was emphasized by the report of the Panel on Large Scale Computing in Science and Engineering, Peter D. Lax, Chairman, [1], which made several recommendations for a national program involving advanced computer technology.

> "Underlying them all is the establishment of a system of effective computer networks that joins government, industrial, and university scientists and engineers. The technology for building networks that allow scientists to share facilities and results is already developed and understood; no time should be lost in connecting existing research groups and computing facilities."

This echoed the conclusions of the report, "Prospectus for Computational Physics," William H. Press, Chairman, [2], which recommended a computing system distributed over a network consisting of principal nodes (with supercomputer capability and large data storage facilities) linked to local nodes (with medium scale computers, advanced graphics devices, array processors, etc.). The Press report stressed the importance of networking the computer facilities and the users.

> "The difference between a computer network and a disconnected set of computers must not be underestimated. A network (and its associated software and human components) provides economies of scale in software development; it allows scientific collaborations on computational projects between

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> participants who are physically remote from each other; it gives the user a choice among a variety of facilities that may be more suitable to his problem than the facility he happens to be physically closest to; it allows researchers at smaller universities to participate on an equal basis with larger institutions. We would not seriously contemplate the establishment of a new initiative in computing for theoretical physics if it did not include the establishment of a supported communication network."

> "There are a number of specific advantages to the distributed picture. Communication costs are, on the average, reduced by placing the physical facilities near the greatest source of their use. The network's total capacity degrades more gracefully under occasional hardware failure, and the probability of catastrophic loss of capacity is reduced almost to zero. There are often observed to be large efficiencies which occur when services such as operator time or software development are provided informally at local nodes at little or no cost (and can then filter out to other nodes). Local management and consulting services, especially when informal and on a small scale, are almost invariably more responsive to special user requirements or situations. Certain requirements (such as graphics processing, three-dimensional displays, and convenient editing on a modern screen editor) require very high baud rates. and so can *only* be implemented efficiently at a local site."

> "The single most important advantage of a distributed network is that it can be changed gradually. It can be increased or decreased in capacity without severe dislocation of most users. It can accommodate changing technological developments without becoming 'locked-in' to a supercomputer of some one particular technological state."

2. Role of the NSF

A national computer network can be envisioned to be analogous to the interstate highway system which supplies the infrastructure necessary for transportation and communication but which leaves it up to the dynamics of the free market to work out which cities will prosper, and what their individual characteristics will be. Similarly, NSF should facilitate the use of the basic channels for computer communication between research institutions and should leave to peer review and local initiative the details of equipping individual sites, and upgrading the network capabilities available to specific nodes. Individual nodes would include large data factories where information is generated either by observation (e.g. VLA, space telescope, Fermilab...) or by computation on supercomputers (e.g. MFECC, NCAR...). Others will be smaller computational or data management facilities, institutional local area networks or clusters of work stations belonging to single research groups.

The objectives of such a network include:

1) providing access by the academic research community to multiple levels of computational resources, including supercomputers;
2) providing access to large data bases;
3) reducing wasteful duplication of effort in software development and encouraging mutual assistance and collaboration among researchers.

In initiating such a national computer network, NSF should work closely with other governmental agencies (DOE, DOD, NASA, Commerce, etc.) which share responsibility for the health of United States' science and technology. These agencies possess unique computing facilities and working networks, which should be important components in any new structure. NSF should be alert to opportunities to work with the national laboratories to provide additional remote computing capability on the network for use by university scientists, and to assist in the transfer of lab software and operating systems to interested universities.

Computer network services are an essential component of the package of actions NSF should take to improve the computing environment for research. This leads to a fourth recommendation:

> **Recommendation 4:** NSF support networks, linking university and laboratory researchers with each other and with supercomputer centers to provide access to facilities, file transfer capability and scientific communication.

F. Advice and Oversight

Since supercomputers are a scarce resource, the allocation of computing resources should be based on need for the speed and memory capacity of supercomputers, efficiency of programs, and scientific justification of research projects. Over the years, the national laboratories have developed useful standard software packages. By sharing these software products with other supercomputer centers, the software development and operational costs of these centers would be minimized. Supercomputer centers should be operated on a cost-effective basis while providing the broad range of computing services required to serve the best science. There are many potential sources for supercomputer services including national laboratories, university computing centers, commercial computer service companies, and others. There are also many possible ways for NSF to support computer services, through individual research grants, purchase of blocks of time, supporting facilities, etc. Network technology is complex and dynamic. Many new services are on the horizon and networks for research must evolve to match changing requirements with available offerings. These concerns are indicative of the large number of policy and technical quesions which NSF must decide in implementing Recommendation 1. Response to them leads to a fifth recommendation:

> **Recommendation 5:** NSF establish an advisory committee to advise the Foundation on policies and mechanisms for supporting computer services for research and to provide oversight.

G. Academic Research in Advanced Computer Systems Design and Computational Mathematics

As shown in Section I. of this report, there are many compelling scientific problems which are beyond the reach of current computing technology. Highly parallel computer systems architectures offer a hope of addressing this need.

The advent of VLSI technology has unleashed great creative energy in academic computer research, especially in the search for new computer architectures. It is now widely believed that computer component technology is nearing the limit of speed allowed by physical principles. Further advances must come from new arrangements of the logical elements into parallel arrays of concurrently acting parts. VLSI technology makes hitherto impossible arrangements practical and offers the promise of 100 to 1000 fold increases in computer speed. Such architectures are radical departures from any we have used before, however, and require new problem strategies, new algorithms, new programming methodologies and new operating systems to make them effective.

Computer companies have shown little interest in pursuing this line of research. Most of the results have come from academia. In the last two years, however, computer and semiconductor manufacturers have formed two consortia to promote longer term research in computer systems and component technology. One, the Semiconductor Research Consortium, Inc. (SRC), is supporting academic research in semiconductor materials, manufacturing technology and circuit design. This will help make the most effective possible components available but the SRC does not intend to support research in computer systems. The other, the Microelectronics and Computer Technology Corporation, (MCC), plans to perform research in several aspects of computer technology including software productivity, packaging, CAD/CAM, and advanced computer systems design. The latter research is expected to include some work on parallel computer architectures but there is no intention of working on the design of high-performance numerical computer systems. The emphasis will be, instead, upon knowledge-based systems, data base management, and human-machine interface.

The planned DARPA strategic computer program addresses parallel architectures in part. It will support certain academic design teams working in concert with industry to build and test machines which incorporate new system concepts. It will be focused primarily on computers for artificial intelligence coupled with rapid access data handling and high speed signal processing, however, and not numerical computation which is a central concern of most scientists and engineers. As a result, it is important for the future of scientific computation that NSF play an active role in the computer design arena by expanding its support of computer research to encompass experimental testing and evaluation of design concepts for numerical computing.

On the other hand, academic researchers have a severe problem in this arena, which is to find the means to carry their computer systems design ideas beyond their desks and simulators through the stage of experimental testing and evaluation. This is an essential step but requires construction of substantial machines and the research on software systems to make them operable. Such projects are difficult in an academic environment and could benefit from industrial engineering and management experience. They are also an order of magnitude more expensive than traditional NSF academic computer research projects because they require team efforts and extensive hardware and software construction.

In closing this discussion, it is important to note that necessary as computer hardware and architecture advances are, there is an essential accompanying role and contribution of research in computational mathematics, algorithms, programming methodology and other aspects of computer science and engineering research. Indeed, past experience has shown that advances in computational capability for aerodynamics, for example, has been due in equal measure to advances in hardware and to new algorithmic approaches or problem solving strategies. Adequate attention must be given to this latter aspect of any substantial computer-related activity. Not only is it necessary that suitable relevant research activity be funded—it is also necessary that a new generation of scientists be trained in appropriate computational mathematics and computer techniques to respond to the current and future needs of this expanding technology. Consideration of all of these program elements leads to recommendation six:

> **Recommendation 6:** Support a vigorous program of academic research and training in the areas of advanced computer systems design, including building and evaluating experimental computer systems, and in computational mathematics, software and algorithms necessary to the effective and efficient use of computer systems.

Entering the area of experimental computer systems research would present some unique problems for research support and management, however. There might be more competing academic projects than money or trained personnel available to carry them to the stage of experimental evaluation. Careful selection would have to be made to assure that only the most significant ideas, measured also against the criterion of constructibility, were selected for further work. In some cases a fusion of separately conceived academic designs might prove to be desirable. During construction, team efforts would be necessary and the use of industrial facilities and expertise would often be advantageous. Early involvement of industry would also promote technology transfer but, on the other hand, imposing proprietary controls on design information too soon would do a disservice to research progress. Finally, it would be necessary to adopt a national perspective in selecting projects for support to assure that the limited financial and personnel resources of the country are appropriately balanced among the diverse interests and priorities of DOD, NSF, DOE, NASA, NIH, industry and the universities.

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IV. A PLAN OF ACTION FOR THE NSF: FUNDING IMPLICATIONS

A. Introduction

The objective of this initiative is to improve computing services for academic research in the U.S. This divides into two subgoals: (a) to improve access to modern computer technology by providing equipment, facilities, services, and networks and (b) to improve computing capability through academic research into advanced computer systems and computational mathematics. NSF has a long history of support in all of these areas through research project support, equipment grants, facilities support, and national centers. Section IV. of this report provides the funding implications of a plan of action for NSF to better meet the requirements of academic science and engineering. Although this plan divides into several parts, they should be viewed as components of a package which, taken as a whole, will improve the use of computer technology for research. Each component is important and none should be asked to stand alone.

It is difficult to gauge the real needs of communities of scientists whose use of computers has been depressed by the obstacles they have had to overcome. As a result, we must depend upon comparisons with other communities which have enjoyed greater resources, insight into the important research problems and opportunities of our time, and knowledge of the research talent in the U.S. The resulting estimates are best judgments of well informed scientists and engineers, no more and no less.

One appropriate comparison is that between typical industrial or national laboratories and typical academic ones. The contrast is striking at all levels of computation services from supercomputers to personal workstations. Academic research productivity is hampered by the present level of computation support. The computation fraction of a typical NSF discipline budget is approximately 3%. It varies among disciplines, of course, being particularly high in the atmospheric sciences which support a major supercomputing facility. Not all research is as computationally intensive as the atmospheric sciences but we should remove the artificial barriers to use of computers in research in all disciplines as much as our resources will allow. It is in this spirit that the following estimates are given.

B. Budget

Note: All figures are given in FY 1984 constant dollars.

1a. Local Facilities

As noted in earlier sections of this report, researchers need a variety of computing services in their normal working environments whether they use supercomputers or not. Support required includes equipment, software, maintenance, local area networks, communication costs, technical support personnel and other costs of computer services than supercomputer time. Some of these facilities will often be used as remote workstations connected to supercomputers but most address the needs for computing which would represent an inefficient use of supercomputers but are essential to the conduct of research. NSF already responds to these needs through its research grants and equipment grants but there is a large gap between the computer support available to academic researchers and that which is considered necessary and is common in well equipped industrial laboratories. It is difficult to estimate the magnitude of this difference but it may be approached by comparing the support provided by NSF in FY 1983 with informed estimates for FY 1984, FY 1985 and FY 1986 of the actual needs of the communities served by the Foundation. The needs include workstations for individuals or small groups of scientists, computer systems for groups of researchers, specialized facilities such as array processors and local area networks. From the estimates given, budget totals for support of local facilities are summarized as follows:

Disciplinary Area	FY83	FY84	FY85	FY86
Engineering	$1.4M	$3.0M	$9.5M	$13.0M
Mathematics	1.2	2.3	6.4	7.3
Physics	2.4	4.1	13.4	10.5
Chemistry	2.1	2.7	4.2	6.4
Materials Research	2.5	3.0	5.2	6.0
Atmospheric Sciences	1.8	3.0	11.0	12.5
Astronomy	1.3	1.5	2.3	3.5
Ocean Sciences	2.5	2.8	3.6	4.5
Earth Sciences	0.8	1.0	1.3	2.5
Computer Research	13.5	16.7	25.0	28.0
Biological Sciences	1.6	2.5	4.1	4.8
Social & Economic Sciences	0.9	1.1	2.3	3.5
Information Sciences	0.2	0.3	0.7	1.2
Behavioral & Neural Sciences	1.3	1.4	1.8	3.0
Total	$33.5M	$45.4M	$90.8M	$106.7M

1b. Supercomputer Capacity

The estimates in Sections I. and III. of this report indicate an immediate need for two supercomputers in addition to NCAR's planned AVC, with growth by a factor of five in two years. As a result, the Foundation should provide two supercomputers for general scientific and engineering research in FY 84 and install eight more, including NCAR's AVC, in the FY 85/FY 86 time period.

Unfortunately, funds available in FY 84 do not allow such a rapid development of this activity. As a result, supercomputer activities in FY 84 will be limited to the purchase of services from one or more existing centers of strength. This will allow a few major research problems to be solved and program development to begin in others.

Cost estimates can be derived from the experience of the DOE, NASA and NSF national laboratories. The data in the Appendix of this report show that annual budgets for these computing centers range from approximately $6M per supercomputer to $16M per supercomputer depending upon the nature and type of other facilities and staff that are associated with the center. They also indicate some benefit from factors of scale, multicomputer centers being less expensive per unit than those which have only one supercomputer.

A supercomputer center should have a fully configured computer system—this improves efficiency as well as offering maximum capability—an adequate staff to operate the equipment efficiently and to assist users, and a complement of auxiliary facilities and services which is appropriate to the type of research computing being done. The NCAR and MFECC models fit well for single discipline centers. They each have two supercomputers with an annual budget of approximately $12M in FY 1984.

On the other hand, multi-disciplinary centers will need larger program maintenance, librarian, and user consulting staffs and, possibly, a broader range of auxiliary equipment. As a result, their costs will be higher. Also, the cost of each center will be critically dependent upon the cost of the central facility which varies from approximately $10M-$15M for currently available systems to an estimated $20M for the next generation systems.

It is clear that there are uncertainties in the actual cost of providing supercomputer services for research but reasonable estimates may be given for the near future based upon present prices. If one assumes a lease/purchase plan, the NCAR-AVC is estimated to cost approximately $6.0M/year. To this must be added staff and other operating costs which, for NCAR, totalled $5.5M in FY 1983. This brings the total to approximately $12M/year/computer for a center with one machine of the class of the NCAR-AVC. Adding a second machine would not double the cost but would increase it to approximately $20M/year for an average of $10M/year/machine. This is a reasonable average cost to use for budget estimates. On this basis and estimating NCAR's computing budget to be $12M in FY 1984 and $19M in FY 1985 if the AVC were to be lease-purchased, we find the following budget totals:

	FY 84	FY 85	FY 86
Total	$14.4M	$70M	$110M

1c. Specialized facilities, e.g., large data banks

These are of concern to individual disciplines or subdisciplines and create an unpredictable requirement. They must be judged in terms of the research priorities at the time the need arises. Although their costs may be substantial and they may require individual accommodation in budget planning, no comprehensive estimate is possible nor is it possible to consider them adequately within this initiative. The costs of these facilities will be included in the budget plans of the disciplines requiring them as the need arises.

2. Networks

Computer networks are an essential component of an initiative to improve computer resources for academic research. They will serve three objectives:

1. provide access by the academic research community to multiple levels of computational resources, including supercomputers;
2. provide access to large data bases;
3. reduce duplication of effort in software development and encourage mutual assistance and collaboration among researchers.

Computer networking technology is already in an advanced state of development and there are many possible sources of data transmission services. NSF requested SRI International, Inc. to make a study of ways to implement computer networking for the academic research community [37]. Cost estimates can be derived from the information provided by that study. Also, DARPA, NASA, DOE and NSF have gained experience operating limited networks. In addition, NSF has discussed future network services with vendors and obtained some cost estimates from them for a hypothetical set of locations in the U.S. Combining all of these inputs, realistic investment in network hardware and software would cost:

	FY 84	FY 85	FY 86
Total	$2.1M	$7.3M	$11.5M

3. Capability—Advanced Computer Systems Research and Computational Mathematics

NSF supports computer systems research and computational mathematics through several programs. The areas of particular relevance to research computing are problem strategies or computational mathematics, algorithms, software systems and software engineering for concurrent processes, programming methodology, and computer systems design. These are supported primarily through the Computer Research Section, several programs of the Mathematical Sciences Section of MCS, the Computer Engineering program of ECSE and the Division of Information Science

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and Technology. Work on problem strategies is also supported through the research programs of all of the disciplines which use computers since some fraction of their investments in computer equipment, computer time, and research personnel results in new computing methodology in the respective disciplines.

A national commitment to computational support for science and engineering calls for increased academic activity in all of these areas. On the other hand, the often cited shortage of faculty and graduate students in computer science and engineering limits the resources which can be usefully invested.

In computer systems research itself, highest priority must be given to work in experimental computer systems including the construction and evaluation of experimental hardware and software for high performance numerical computing. A program for this purpose has been described in the Lax report ([1] p. 42-76) where it is recommended that up to five construction projects be supported at any one time. Each project is estimated to cost $5M/year.

Taking all of the elements in this area of research together, a budget plan appropriate to the needs is:

	FY 84	FY 85	FY 86
Experimental Computer Systems .	$1.5M	$11.5M	$23.0M
Other Related Computer Research and Computational Mathematics	$6.5M	$8.5M	$10.0M
Total	$8.0M	$20.0M	$33.0M

4. Summary

The total initiative is summarized below:

	FY 84	FY 85	FY 86
Local Facilities	$45.4M	$90.8M	$106.7M
Supercomputers	$14.4M	$70.0M	$110.0M
Networks	$2.1M	$7.3M	$11.5M
Advanced Computer Systems and Computational Mathematics ...	$8.0M	$20.0M	$33.0M
Total	$69.9M	$188.1M	$261.2M

C. Implications for NSF Organization

Of the several activities proposed in this initiative, the support of local facilities and of experimental computer architecture research fit well within existing NSF programs. The support of supercomputer and networking services may not. A key question in considering this issue is the nature of the supercomputer facilities. Should they be single-purpose or multidisiplinary? Should they be located on university campuses or at national centers in the manner of NCAR? There are arguments for each point of view.

1. Discipline-Oriented Facilities

Discipline orientation would concentrate scientists with common scientific interests at certain shared facilities. This would encourage discourse and mutual assistance because of the commonality of experience and interests. It would also simplify the problem of peer review of applications for use of the supercomputer facilities because only problems from closely related fields would be under consideration. NCAR experience with this type of operation has been good. It is also argued that universities cannot manage large computing facilities for research well and, as a result, they should be placed in special institutes or national centers.

Another advantage of this approach is that it maps easily onto the organizational structure of NSF. On the other hand, few NSF staff have the technical competence to evaluate supercomputer or networking proposals and exercise oversight.

2. Multidisciplinary Facilities

Some scientists, e.g., Professor Kenneth G. Wilson, Cornell University, assert quite emphatically that computer facilities organization should not reflect discipline. His argument is that in computing, attention is on the mathematical and computing methodology as well as the scientific motivation and there is much to be gained by the cross-fertilization of different intellectual backgrounds among persons having common computing interests. It is for this reason that Professor Wilson is planning an interdisciplinary institute of theoretical research at Cornell. This commonality of methodology across widely disparate scientific applications is highlighted in a forthcoming study of the National Research Council [31] which analyzes several scientific problems from the viewpoint of the mathematics and computing algorithms involved.

Proponents of this view argue, further, that this interdisciplinary organization fits well in a university environment and, because of the urgent need to train students, facilities should be placed on university campuses where they can be accessed by students and where students can share in the cultural environment of high speed computing. They argue further that if universities were given full support for supercomputer facilities so they would not have to justify them by their value to undergraduate education, the competing interests which have interfered with good management of computers for research in the past would not be present.

From this point of view, supercomputer and networking services are related activities, central to the research interests of all of the research directorates. They are similar in some respects to the services provided years ago by the Foundation's computer facilities program or to the synchrotron radiation facilities of today which serve chemistry, biology, and materials research.

These two examples suggest that NSF support of these activities might be centralized in one place, for example, an Office of Computing Resources, but that the specific location of that office in the organization chart of the Foundation should be of secondary importance. The office should not seem to be the captive of one interested discipline but it should be integrated with the research directorates that it serves. It should coordinate with all of the research disciplines but not interfere with already established and effective responsibility for computer activities such as AAEO's responsibility for NCAR. These criteria and the intended functions suggest creating an Office of Computer Resources reporting either to one of the research assistant directors or to the Director.

It seems probable that the impact of these questions on NSF organization is a serious concern only during a transition period from little support of large-scale computing to extensive support. If large-scale academic computing were commonplace, there would probably be a mixture of discipline oriented and interdisciplinary facilities supported by NSF. Many NSF staff would be well versed in the culture of large-scale computing and the problems of resource allocation, proposal evaluation, and oversight could be easily shared among the research directorates. None of those hypotheses apply today, however, and the Foundation could easily impose its organizational structure on large-scale computing activity. This would be a disservice to science because we do not have reason to believe that NSF's structure applies well to computational science. For this reason, until large-scale computing grows to its natural stature in research, an office addressing large-scale (but not local) computer and networking services for all of the disciplines may be advisable.

Selected Bibliography

1. "Report of the Panel on Large Scale Computing in Science and Engineering," sponsored by DOD and NSF in cooperation with DOE and NASA, Peter D. Lax, Chairman, December 26, 1982.
2. "Prospectus for Computational Physics," Report by the Subcommittee on Computational Facilities for Theoretical Research to the Advisory Committee for Physics, Division of Physics, National Science Foundation, March 15, 1981, William H. Press, Chairman.
3. "Future Trends in Condensed Matter Theory and the Role and Support of Computation," report by the Condensed Matter Theory Panel, published under the auspices of the council on Materials Science for the Division of Materials Sciences, U.S. Department of Energy, J. D. Joannopoulos and A. N. Berker, Co-Chairman, September 22, 1981.
4. "The Numerical Aerodynamic Simulator—Description, Status, and Funding Option;" a report prepared at the request of the Committee on Commerce, Science, and Transportation, United States Senate; Dec. 1981, NASA.
5. Numerical Aerodynamic Simulator; Background, Requirements, and Justification; NASA, Ames Research Center, Revised January 1982.
6. "Simulation of Turbulent Shear Flows: What can we do and what have we learned?" presented by invitation at the Seventh Biennial Symposium on Turbulence, Rolla, MO, by W. C. Reynolds, Department of Mechanical Engineering, Stanford University, September 21, 1981.
7. "A Commentary on Computational Mechanics," J. E. Oden and K. J. Bathe, Applied Mechanics Reviews *31* (1978) pp. 1053-1058.
8. "Report on the Utilization of Large Scale Computers," Committee on the Utilization of Large Scale Computers in ASGA, Bennett Miller, Chairman, July 1, 1977.
9. "Nuclear Weapons and Computers, Summary: The Role of Large Scale Computers in the DOE Nuclear Weapons Program," the Gold Report, prepared for the Director of Military Applications, U.S. Department of Energy, March 1978.
10. "DOE Research in Utilization of High-Performance Computers," B.L. Buzbee, W. Jack Worlton, G.A. Michael, G. Rodrigue, LA-8609-MS, Los Alamos National Laboratory, December 1980.
11. "A Philosophy of Supercomputing," Jack Worlton, LA-8849-MS, Los Alamos National Laboratory, June 1981.
12. "Department of Energy FY 1983-1987 ADP Long Range Plan," Office of ADP Management, December 1981.
13. "An Assessment of Trends in the Solid State Sciences," National Research Council, July 1980.
14. "Long Range Plan for Nuclear Science," excerpts from a report by the Nuclear Science Advisory Committee, July 30-August 4, 1979.
15. "Draft II—Astronomy Survey Committee: Report of the Panel on Data Processing and Computational Facilities," May 19, 1980.
16. "Workshop on Computational Astrophysics," NASA Ames Research Center, February 1980.
17. "Magnetic Fusion Energy and Computers: The Role of Computing in Magnetic Fusion Energy Research and Development," Office of Fusion Energy, DOE, October 1979.
18. "Report by the Subcommittee on Computational Capabilities for Nuclear Theory to the DOE/NSF Nuclear Science Advisory Committee," December 1981.
19. "Universities and the Future of Technology Development," Kenneth G. Wilson, Laboratory of Nuclear Studies, Cornell University, Ithaca, New York.
20. "A Data Flow Supercomputer," Jack B. Dennis, G-R Gao, Kenneth W. Todd, Computation Structures Group Memo 213, MIT Laboratory for Computer Science, Cambridge, Massachusetts, March 1982.
21. "Foreign Travel Trip Report: Visits with Japanese Computer Manufacturers," R. Ewald, Bill Buzbee, J. Worlton, CDO/82-6782A, Computation Division, Los Alamos National Laboratory, April 5, 1982.
22. "Supercomputers," Ronald D. Levine, Scientific American, January 1982.
23. "An Assessment of Computational Resources Required for Ocean Circulation Modeling," Ad Hoc Committee on Computing Resources and Facilities for Ocean Circulation Modeling, Ocean Sciences Board, Commission on Physical Sciences, Mathematics and Resources, National Research Council of the National Academy of Sciences, 1982.

24. "Nearest Neighbor Concurrent Processor," E. Brooks, G. Fox, R. Gupta, O. Martin, S. Otto, E. De Benedictis; California Institute of Technology, DOE Research and Development Report, CALT-68-867, September 1981.

25. "Why the U.S. Government Should Support Research On And Development Of Supercomputers," Bill Buzbee, Los Alamos Report LA-UR-82-1968, July 1982.

26. Los Alamos SCIENCE, Los Alamos National Laboratory, Vol. 2, No. 2 (1981).

27. Justification for Class VI Scientific Computing Capability at Sandia Laboratories, Albuquerque; Sandia Laboratories, February 1979.

28. "Trends and Pacing Items in Computational Aerodynamics," D. R. Chapman, Lecture notes in Physics, 141, Springer-Verlag, 1981.

29. "Scientific Justification for an Advanced Vector Computer," National Center for Atmospheric Research. Prepared for NSF by the University Corporation for Atmospheric Research, December 1982.

30. "The Influence of Computational Fluid Dynamics on Experimental Aerospace Facilities: A Fifteen-Year Projection." Prepared by the Committee on Computational Aerodynamics Simulation Technology Developments, Aeronautics and Space Engineering Board, Commission on Engineering and Technical Systems, National Research Council, 1983.

31. "Computational Modeling and Mathematics Applied to the Physical Sciences" A report prepared by the Committee on the Applications of Mathematics, Office of Mathematical Sciences, Commission on Physical Sciences, Mathematics and Resources, National Research Council, to be published.

32. "Research Directions in Computer Engineering" Report of a Workshop, Herbert Freeman, ed., Technique et Science Informatiques, 1982, pp. 423-432.

33. "Supercomputers: Foreign Competition and Federal Funding" Issue Brief Number IB 83102, Nancy Miller, Library of Congress, Congressional Research System, June, 1983.

34. "Doing Physics with Computers," Special Issue of Physics Today, May, 1983.

35. "The National Resource for Computational Chemistry, Phase I: Evaluation and Recommendations," Report of an Ad Hoc Review Committee, Oak Ridge National Laboratory, ORNL/TM-7294, May, 1980.

36. "The Fourth Inventory of Computers in Higher Education: An Interpretive Report," John W. Hamblen and Carolyn P. Landis, EDUCOM Series in Computing and Telecommunications in Higher Education 4, 1980.

37. "USERNET: A Preliminary Architectural Study and Implementation Strategy," Final Report by Franklin F. Kuo et al, SRI International, Inc., June 1983.

APPENDIX

LARGE SCALE COMPUTING FACILITIES

NATIONAL SCIENCE FOUNDATION

NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

Major Systems Currently in Place

- 2 CRAY-1A's (1 Megaword Main Memory each)
- 2 IBM-4341 Interactive Computers
- Ampex Terabit Memory Mass Store (75 x 10^9 bytes of on-line storage)

Research Community Served

- 90% Atmospheric Science, 9% Ocean Sciences, 1% other
- NCAR and Atmospheric and Related Scientific Areas in Academia
- 850 Users

Communication Systems for Remote Users

- Uninet Packet Switching Services (1200 bps)
- Dial-up Telephone Access (300/4800 bps)
- Dedicated Leased Telephone Lines (2400-4800 bps)

Budget/Staff/Charges

- No charge for NSF-Supported efforts; $2200 per prime CPU hour for others
- $7.5M FY 1983 Budget-$2.0M Capital Facilities for 2nd CRAY-1A; $5.5M Operating Budget
- Staff of approximately 100

Plans

- FY 1984-New Mass Store System ($3M)
- FY 1985-Class VII Computer System (also to serve ocean scientists) ($20M)
- FY 1986-Wide-Band communications ($17M)

NATIONAL MAGNETIC FUSION ENERGY COMPUTER CENTER

Major Systems

- CRAY-1 (1 Megaword Main Memory); CRAY-1S (2 Megaword Main Memory)
- CDC 7600
- CDC 38500 Mass Store (62,500 Megabytes of storage, retrieval time is 10 sec.)

Research Community Served

- 95% to Magnetic Fusion Energy Research Community
- 5% to Other Energy Research
- 2,000 Users

Communication System for Remote Users

- Dual 56K bps Satellite System with 4 Remote User Service Centers
- Dial-up Service through TYMNET, ARPANET, Commercial, or FTS
- Dedicated Leased Telephone Lines (4800 bps)

Budget/Staff/Charges

- No Charge
- $12.5M FY 1983 Operating Budget (Includes lease of 1 CRAY)
- Staff size approximately 85

Plans

- Class VII Computer System in FY 1984
- Another Class VII System in FY 1987
- Modest Expansion of Mass Store in FY 1984

LOS ALAMOS NATIONAL LABORATORY

Major Systems

- Access Partitioned into Three Levels: Administrative, Secure, Open
  - Open: 1 CRAY, 3 CDC 7600's 1 CYBER 825
  - Total: 5 CRAY's, 4 CDC 7600's, 3 CYBER 825's
- IBM 3850 Mass Store Cartridge System (1.2 trillion bytes, 85% returned in 5—10 secs.)

Research Community Served

- Government Agencies, Laboratories, and Non-Profit Institutions
- 4400 total Users

Communication System for Remote Users

- Dial-up Telephone Access through Arpanet, Telenet and Commercial Lines (300/1200/2400 bps)

- Dedicated Leased Telephone Lines (Up to 5600 bps)
- Magnetic Fusion Energy Network (56K bps)

Budget/Staff/Charges

- $39M Budget for FY 1983
- Staff of 240 FTE's
- $636 charge for each prime time CRAY CPU hour. Also there are charges for Connect Time, Ports, Storage, Output.

Plans

- Install Denelcor HEP-1 Experimental System in FY 1983
- Upgrade a CRAY-1 to a CRAY-XMP in early FY 1984
- Add 3 Class VII Systems (FY 1985-1988)
- Upgrade Mass Store System in FY 1984, FY86, FY88

NASA—AMES RESEARCH CENTER

Major Systems

- CRAY—1S (1 Megaword Main Memory; 16 Megaword Solid State Disk Memory comparable in response time to Main Memory)
- CDC—7600

Research Community Served

- Computational Fluid and Aerodynamic Community*
- In-House Computational Chemistry, Astrophyssics, Stratospheric Modeling and Image Processing Communication for Remoter Users
- 500 Users

Communication System for Remote Users

- Dial-up Commercia and FTS Telephone Lines (300/1200 bps)
- Arpanet (3-6 Kbps)

Budget/Staff/Charges

- FY 1983 Budget at $9.0M with a staff of 100+
- No direct charges to NASA grantees
- NASA donates time for cost sharing purposes on projects of joint interest with other agencies
- $2,000/normal priority CPU hour for CRAY; $750/normal priority CPU hour for 7600

Plans

- Mass Store System in FY 85; Upgraded to maximum configuration in FY 87
- Upgrade CRAY-1S to CRAY-XMP in FY 84
- FY 87 goal of serving the Computational Fluid & Aerodynamics Community with:
  - — 2 Class VII Computers
  - — 1 Class VI Computer (enhanced)
  - — Remote Users Acessing Systems through Satellite-Based Sending and Receiving Communications

NASA—GODDARD

Major Systems

- CYBER 205 (2 Pipelines, 1 Megaword Main Memory)
- IBM 3081
- Amdahl V6, V7B
- Masstor 861 Cartridge System (100 billion bytes; access time a few seconds)

Research Community Served

- NASA-Goddard Scientists
- NASA-Funded Researchers Working in Earth Science Observations
- Researchers working with NASA on common areas of interest
- 1000 users

Communications for Remote Users

- Dial-up telephone lines (300—4800 bps)
- Dedicated leased telephone lines (up to 4800 bps)

Budget/Staff/Charges

- $10M FY 1983 Budget (Capital and Operating Costs)
- Staff of approximately 60 FTE's
- No direct charges to NASA grantees working on Earth Observations
- To others, the charges are approximately $1000/CPU hour for the CYBER 205, and $500/CPU hour for the IBM 3081. In the future there may be charges for Connect Time, Storage and Output.

Plans

- Node on NASA Wide-band Communications System Linking Large NASA Computers
- Massively Parallel Processor (MPP)
  - — 128 x 128 Array Processor; 10 Million Instructions/Sec.
  - — Built under Contract with Goodyear Aerospace
  - — Cost under $7M
  - — To be delivered in late FY 1983

NASA—LANGLEY

Major Systems

- CYBER 203—(1 Megaword)

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* In conjunction with joint research activities conducted at NASA-Ames.

- CYBER 730, CYBER 170's, CYBER 750
- Masstor 860 Cartridge System (80-100 billion bytes of storage)

Research Community Served

- NASA-Langley Research Scientists
- NASA-Funded Researchers working in structures, strength of material, aeronautics and space, and atmospheric modeling
- 250 Users on CYBER 203; 2000 overall

Communications for Remote Users

- Dial-up telephone lines (1200) bps

Budget/Staff/Charges

- $16M for FY 1983
- Staff of approximately 350
- Charge $1300 per CYBER 203 CPU hour

Plans

- Upgrade Memory on CYBER 203 to 32 Megaword
- 50 Megabit Local Communication Network Langley

NASA-LEWIS

Cleveland, Ohio

Contact: Dr. Ford, Director for Scientific Computing

Major Systems Currently in Place

- CRAY 1S; in place 9 months; used at 50% capacity
- IBM 3033—370 (attached processor)
- UNIVAC 1100/42

Research Community Served

- Theoretical and experimental scientists and engineers
- Mostly aerodynamics and related fields
- Available to NASA LEWIS scientiists and engineers, other NASA Centers, NASA contractors, other government agencies, and a few universities

Communication System for Remote Users

- Dial-up telephone access
- Dedicated leased telephone lines
- CAT TV cable—main access, very broadband cable, 8 megahertz, allows great variety of networks

Budget/Staff/Charges

- Free for NASA-supported efforts
- No formal mechanism for charging "other" users; there will be one in place shortly; ballpark figure of $1,000/hour
- 2,500 people employed at computer center of which approximately 1,500 are regular users
- FY 1983 computer center budget-larger than NCAR

Plans

- Acquire two new scientific computers and one new computer for business and information management; IBM 3081's
- Plans to upgrade memory
- No plans to acquire another supercomputer

COLORADO STATE UNIVERSITY

— Leasing a CYBER 205 ($2.3M/Year)
  - 2 megaword central memory
  - 2 vector pipelines
  - CDC 819 mass store system (3 billion bytes of on line storage)
  - Cost for university users is $2000 per hour

— CDC Contributions
  - Purchased $1.7M worth of CPU time
  - Distributed time to 30 individual scientists from 22 universities for independent scientific research

— Examples of Research Projects using CYBER 205 are:
  - Petroleum Engineering & Reservoir Analysis Problems
  - Subsurface Geological Mapping
  - DNA Modeling
  - Monte Carlo Techniques Applied to Plasma Physics

— Access
  - Dial-up telephone lines
  - CSU Network—dedicated lines

U. of Mass	14.4 Kbps
Dartmouth T.S.	9.6 Kbps
National Bureau of Standards	9.6 Kbps
Solar Energy Research Institute	9.6 Kbps
Several Petroleum Research	9.6 Kbps

Companies and Centers

- National Bureau of Standards

  Working agreement for NSB researchers in mathematics and computer science

- 20% of CPU utilized

UNIVERSITY OF MINNESOTA

- Leasing CRAY 1A, $1.56M/year
  - 1M words of memory (maximum capacity)
  - 3 disc drives
  - Used at one-third of real capacity
  - Front-end disc capacity of over 12 gigabytes
  - Front-end interactive computers: VAX 11/780 and CYBER 730
- CRAY Contributions
  - System purchased at a $2M discount
  - 5 years maintenance at nominal changes
  - CRAY Inc. is allotted the night shift (7 hrs.) for development work
- Cost of Services:
  - Internal rate—at $2,000/hr.—available to university personnel, federal, and state government and other non-profit organizations
  - External rate—mainly to local high-tech industries—50% mark-up ($3,000/hr.)
  - Available to EDUNET network
  - The above rates subject to substantial discounts (as high as 50%) for high-volume users
- Examples of Research Projects
  - Chemical engineering—phase changes in material
  - Petroleum recovery
  - Finite element computation
  - Image processing—animated movies involving the studies of molecules
  - Economic modeling
- Future Plans
  - Replace front-end
  - Proposal to form a consortium with four industrial users for a one-fifth share in a CRAY XMP until a CRAY II is available
- Access
  - Dial-up telephone lines
  - Dedicated lines 1200 Bps, 4800 Bps, 9600 Bps, 19.2 Kbps

PURDUE UNIVERSITY

- Acquired a CYBER 205 for $5.5M
  - Funding from University and State of Indiana
  - 1 megaword central memory, 2 vector pipelines
  - At the moment, there are a limited number of production runs; much work is occurring on software and systems development, approximately 6 CPU hours per day are available to users
- CDC Contributions
  - Purchased $1.5M worth of CPU time for computer-aided design research
- Plan for Enhancement
  - Increase memory to 2M words ($2.3M)
  - Add 2 high speed channels, disk and tape systems, graphics systems ($1.8M)
- Some examples of research projects
  - Biological molecular structures
  - Solar cells
  - Mesoscale storm models
  - Chemical molecular dynamics
  - Solution of certain elliptic PDE's
- Establishing a Center for Vector and Parallel Computing
  - Research in algorithms and software for Vector and Parallel Computing

BOEING COMPUTER SERVICES

- Owns CRAY 1S
- Used at 50% capacity
- Direct dial-up lines
- Dedicated lines

CYBERNET

- Acquired CYBER 205
  - time sharing option
  - cost depends on type of work load
  - types of applications include weather predictions and nuclear codes
  - dial-up telephone lines
  - use at one-half full capacity

UNITED INFORMATION SERVICES

- Own CRAY 1S
- Time sharing and batch
- Applications include high-tech companies, business, i.e. insurance groups
- Cost depends on I/O units used and type of peripheral equipment
- Dial-up lines
- Dedicated 1200 bps—9600 bps

CORNELL

Equipment

IBM 370-168, several 4341's (central campus facility), IBM 3081 being installed
FPS AP-190L Array Processor
FPS-164 Attached Processor

No. of users (Aray and Attached Processors) 50-100 direct, available to 2000 general users

Costs

Array Processors: capital costs: $0.5M

Array Processor operating expenses and support costs: $150K/yr, staff of 3+ (120 in Computing Center)

Array Processor typical rates: $20-$40/CPU hr non-profit $75/hr external

Scientific computing charges on IBM hosts: $500-1500/hr on IBM 370/168 Computing center budget $10M

Access available through TELENET, TYMNET, BITNET.

Aims

Cornell measures the success of its scientific computing facility by the quality of research that *individual faculty members* achieve using the facility. At present a consortium of four faculty research groups are the primary focus of the scientific support effort:

Keith Gubbins (chemical engineering, molecular dynamics)

Stu Shapiro and Saul Teukolsky (astrophysics and general relativity, fluid dynamics, particle dynamics)

Kenneth Wilson (high energy physics, critical phenomena, Monte Carlo simulations)

G. Chester, N. Ashcroft, J. Wilkins, (solid state physics):

The computing capability available to ***each one*** of these four research groups is approximately 2,000 hours/year of processor time, which is competitive with the capabilities ***per research group*** supplied at major national facilities.

Future Plans

Obtain a 4000 Array Processor facility, organized with high speed parallel interconnects between processors, to achieve 30-100 Gigaflop* capability. Target date: Fall 1986

One or two 64 processor facilities to be acquired earlier for benchmarking.

A joint Cornell-computing industry proposal to realize these plans should be ready by Fall 1983.

This facility will provide a desperately needed thousand-fold increase in capability for leading-edge research projects at Cornell.

In addition a distributed supercomputing network of supermini computers, attached processors, and other high-performance systems is being established to expand Cornell's capacity at present levels of capability. The aim is to serve the entire theoretical science, theoretical engineering and theoretical agricultural communities at Cornell, totalling some 500 individuals.

Also, use will be made of national facilities, starting with the Goodyear MPP at NASA Goddard Laboratory.

Emphasis will continue to be on development of new, cost-effective approaches to Scientific Computing.

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* 1 Gigaflop = 10^9 arithmetic operations/second

END

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